

NASA SCIENCE MISSION DIRECTORATE

*Earth-Sun System Applied Sciences Program
Air Quality Program Element*

Benchmark Report:

Globally Assimilated Lateral Boundary Conditions
Improve CMAQ Ozone Estimates

September, 2005



*Expanding and accelerating the realization of economic and societal
benefits from Earth-Sun System science, information, and technology*

NASA Earth-Sun System Applied Sciences Program

Globally Assimilated Lateral Boundary Conditions Improve CMAQ Ozone Estimates

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NASA Earth-Sun System Applied Sciences Program

Globally Assimilated Lateral Boundary Conditions Improve CMAQ Ozone Estimates

Overview

This report describes work completed in partnership between NASA and US EPA to modify the widely used decision support tool, the US EPA's Models-3/Community Multi-scale Air Quality Model (CMAQ), to accept time- and spatially-varying lateral boundary conditions, to conduct evaluations, and to analyze the effect of this modification on CMAQ's performance.

US EPA's Models-3/CMAQ modeling system ((Byun and Ching, 1999; Byun 1999a, Byun 1999b) is a "one-atmosphere" modeling system designed to approach air quality as a whole by including state-of-the-science capabilities for modeling multiple air quality issues, including ozone, particulate matter, visibility degradation, acid deposition, and air toxics, at multiple scales. The EPA uses Models-3/CMAQ as an underlying Decision Support System (DSS) in the development of air quality regulations and strategies. The model is used to provide predicted pollutant concentrations, including ozone, for current and future air quality control strategies, providing the necessary quantitative information as a basis for EPA, Regional Planning Organizations, and State and Local mitigation strategies for reducing ozone, particle pollution and regional haze.

Many of the pollutants modeled within CMAQ are spatially inhomogeneous and have a regional or local nature because of their chemical reactivity and emission sources; however, research is increasingly showing continental and hemispheric contributions. The CMAQ model was developed for regional scale domains; however, linkages to global scale information is needed to account for these larger scale contributions. Such inputs from global models can provide more realistic and accurate descriptions of influx of pollutants, and provide a means to account for the contributions of pollutants transported over larger distances.

The goal of this project was to determine if a multi-scale modeling and data assimilation framework for constraining global model predicts improves the prediction of large-scale transport and local productions of surface ozone and overall model performance. The approach is to provide lateral boundary conditions generated from a global model output to CMAQ.

Benchmark Intent

This activity supports US EPA's ongoing mission to bring sound science to its decision making. NASA satellite observations of Criteria Pollutants have been scientifically validated through NASA processes. The NASA-EPA partnership identified this activity as high priority in a series of scientist-to-scientist exchanges. The Benchmark process is NASA's mechanism for accountability of this activity. The task plan is fully aligned with the Air Quality program Element Plan and its short term objectives.

Short-term Objectives (FY05)

| | |
|------------------------|--|
| QIII - QIV 2005 | Complete transition of MODIS Aerosol Optical Depth (AOD) technique to NOAA & EPA for air quality forecasting. Complete validation & benchmark reports on the transition, improved techniques, and benefits. |
| 5ESA2, 5ESA6, 5ESA7 | Validate and complete benchmark report on NASA science support to boundary conditions for CMAQ (e.g., EP-TOMS Ozone residuals, assimilations, and boundary conditions (BC) from RAQMS). |
| QIII - QIV 2005 | Establish agreements with at least one federal partner and at least one non-federal partner or international organization (e.g., Regional Planning Organizations). |
| 5ESA2, 5ESA6, 5ESA7 | Establish joint development plan with EPA, NOAA on NASA science support (e.g., Terra, Aqua, Aura, CloudSat, RAQMS, GOCART) to air quality tools (e.g., AIRNow AQI, CMAQ, WRF-CHEM), including emissions inventories. |

Approach

This project was designed to benchmark the use of multi-scale modeling and chemical data assimilation of air pollutants as an improvement to the CMAQ modeling of large scale transport and local production of ozone.

Global and regional air quality is linked through complex interactions between highly heterogeneous surface emissions, local radical chemistry, boundary layer exchange processes, enhancements in background levels of ozone and its precursors, and long range transport. A global chemical data assimilation system can constrain regional air quality models and can provide a link between global and regional air quality. In this case, we assimilated global ozone column data from the satellite Earth Probe TOMS, and global solar occultation (stratospheric limb) ozone measurements from the satellite based instruments HALOE, POAM, and SAGE, during the period of June 15- July 15, 1999. Both stratospheric profile and total column ozone observations are required to produce physically consistent ozone distributions. The benchmark time period included an air quality field study, the US 1999 Southern Oxidant Study (SOS 99), which provided additional detailed ozone measurements for comparisons.

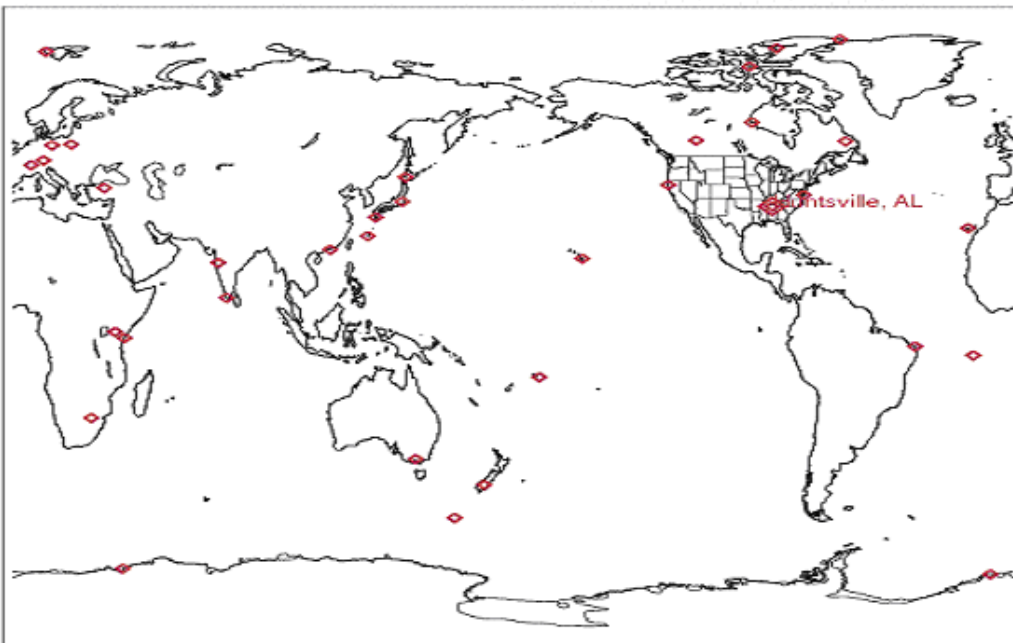
Two global ozone assimilation frameworks were considered, the NASA LaRC-University of Wisconsin Regional Air Quality Modeling System (RAQMS) [Pierce et al., 2003] and the NASA GSFC Finite Volume Data Assimilation System (FvDAS) [Stajner et al., 2004].

RAQMS is a unified (stratospheric and tropospheric), multi-scale (global to regional) air quality modeling/data assimilation system with online chemistry. The statistical digital filter analysis system [Stobie 1985, 2000] is used within RAQMS to perform a univariate assimilation of stratospheric profile and total column observations of ozone. RAQMS was used to evaluate the feasibility of assimilating high vertical resolution, but spatially sparse solar occultation profile combined with total column ozone measurements.

The resulting ozone analyses were compared to FvDAS ozone analyses based on observations from the Solar Backscatter UltraViolet/2 (SBUV/2) instruments, which have been assimilated in

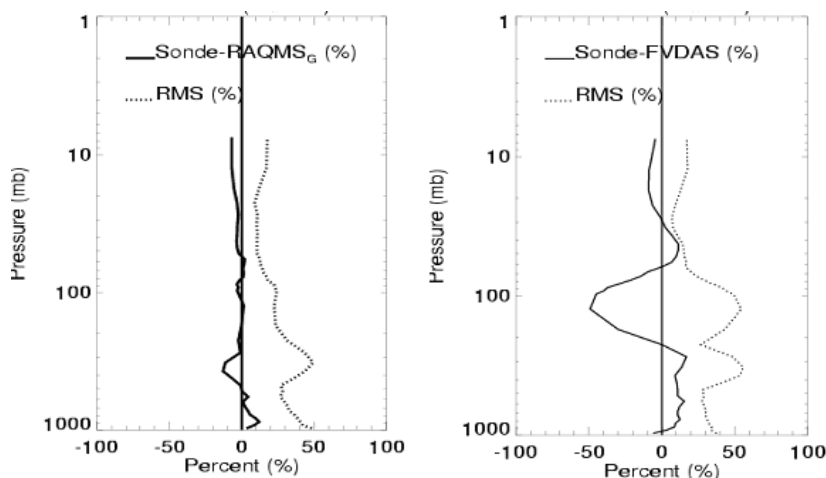
near-real time at NASA's Data Assimilation Office since January 2000 [Stajner et al. 2004]. To be consistent in this evaluation of assimilation frameworks, RAQMS used meteorological analyses from FvDAS. FvDAS (no online chemistry) used 24-hour averaged ozone production and loss terms from the RAQMS runs. We compared results from these two assimilation frameworks with World Meteorological Organization ozonesonde measurements (Figure 1a).

Figure 1a. Locations of the World Meteorological Organization ozonesonde sites used in the global ozone assimilation framework evaluation.



The comparison of the two assimilation frameworks is presented below in Figure 1b. The assimilation of solar occultation data within the RAQMS analysis system reduced biases in the lower stratosphere/upper troposphere relative to assimilation of SBUV measurements within FvDAS. Therefore, we used the RAQMS ozone analyses for this benchmark study.

Figure 1b. Statistical comparison between World Meteorological Organization ozonesondes, RAQMS (left), and FvDAS (right) ozone analyses for latitudes north of 30 degrees north. Mean % biases (solid) and RMS % errors (dotted). RAQMS mean bias is lower than FvDAS mean bias, and integrated RAQMS RMS error is less than FvDAS RMS error.



The RAQMS global ozone assimilation provided variable lateral boundary conditions at each of the four sides of the continental North America domain for this benchmark. US EPA provided the baseline assessment run (CMAQ /baseline) for the selected time period.

The overall study comprised the following activities:

1. obtain US EPA approval of the modification of CMAQ to accept time and spatially varying boundary conditions,
2. verify the performance of CMAQ in that configuration.
3. perform model runs with assimilated boundary conditions in the modified CMAQ.
4. evaluate the model's performance with respect to the baseline runs and with respect to "truth" observations (from EPA AIRNOW surface sites and World Meteorological Organization ozonesondes).
5. analyze the differences between the CMAQ/baseline and CMAQ/RAQMS runs.
6. determine the value of time varying boundary conditions for this Decision Support Tool.

Methods

The techniques, models, and data used in this benchmark work are described in the literature [Song et al., 2005]. US EPA identified the University of Houston collaborators as acceptable partners for modifying the US EPA tool, CMAQ. In the following discussion, "CMAQ" refers to the University of Houston modified CMAQ.

Verification of University of Houston CMAQ Modifications

Prior to initiating this study, we confirmed that the unmodified University of Houston CMAQ version 4.3 adequately represented the unmodified US EPA CMAQ baseline results produced by the US EPA collaborators. [The ratio of the maximum difference between the two unmodified

versions of CMAQ to each maximum concentration of each species fell within the range of 10^{-2} , and the ratio of the maximum difference to each mean concentration is smaller than 10^{-4} .] Therefore, UH CMAQ was judged acceptable for further studies to benchmark CMAQ performance with lateral boundary conditions provided by RAQMS assimilation of satellite data.

CMAQ results with the lateral boundary conditions generated by RAQMS

In order to benchmark the performance of CMAQ with and without assimilated boundary conditions, it was first necessary to modify CMAQ version 4.3 to accept assimilated boundary conditions provided by RAQMS. We created and evaluated the RAQ2CMAQ tool to link global RAQMS output with CMAQ. RAQ2CMAQ consists of input/output routines, conversion between two grid domains, and mapping of chemistry, and the vertical interpolating process. The species mapping between the RAQMS chemical mechanism and CMAQ Carbon Bond 4 (CB4) is summarized in Appendix A.

We conducted two CMAQ model runs (one with the baseline boundary conditions, and one with RAQMS assimilated boundary conditions) for the June 15- July 15, 1999 period. Figure 2a provides results from this comparison. Moderate increases in surface ozone mixing ratios over the mountainous regions of the western US, and significant increases in ozone mixing ratios in the upper troposphere were seen when the RAQMS assimilated boundary conditions were included in CMAQ.

Figure 2a. Mean ozone differences (ppbv) between CMAQ/baseline and CMAQ/RAQMS observed near the surface ($\sigma=0.9980$). At the surface, use of assimilated boundary conditions (CMAQ/RAQMS) results in surface ozone increases of 4-8 ppbv over the western mountains, and reduction of up to 12 ppbv over the northern (Canadian) boundary and 18 ppbv over the western (Pacific) boundary.

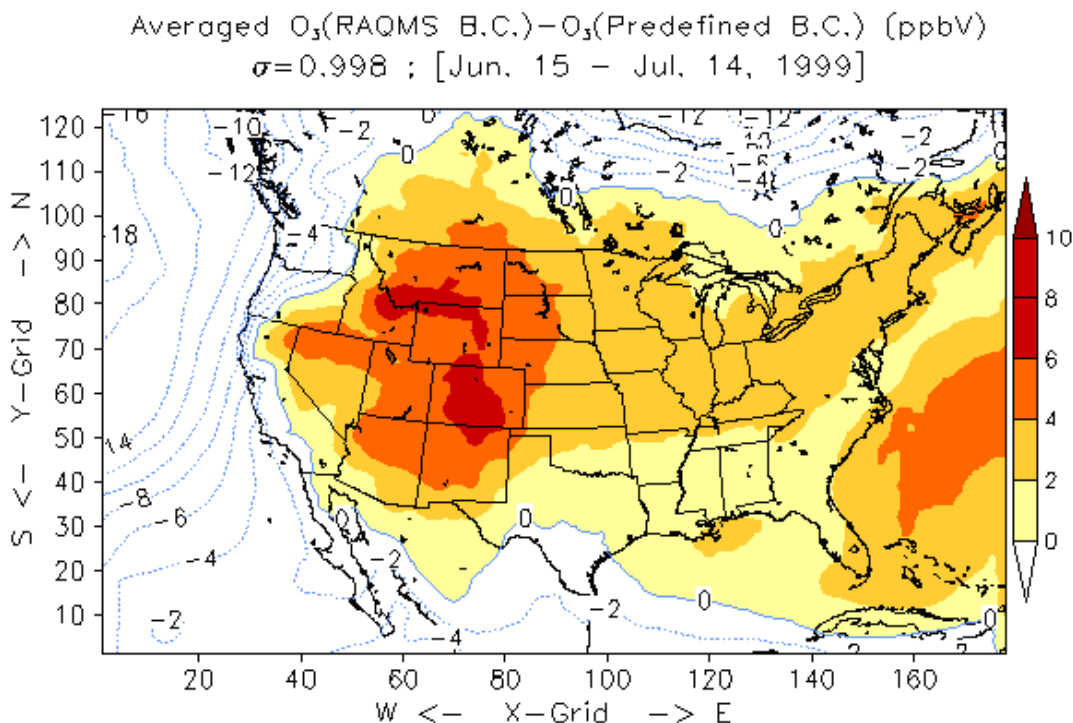
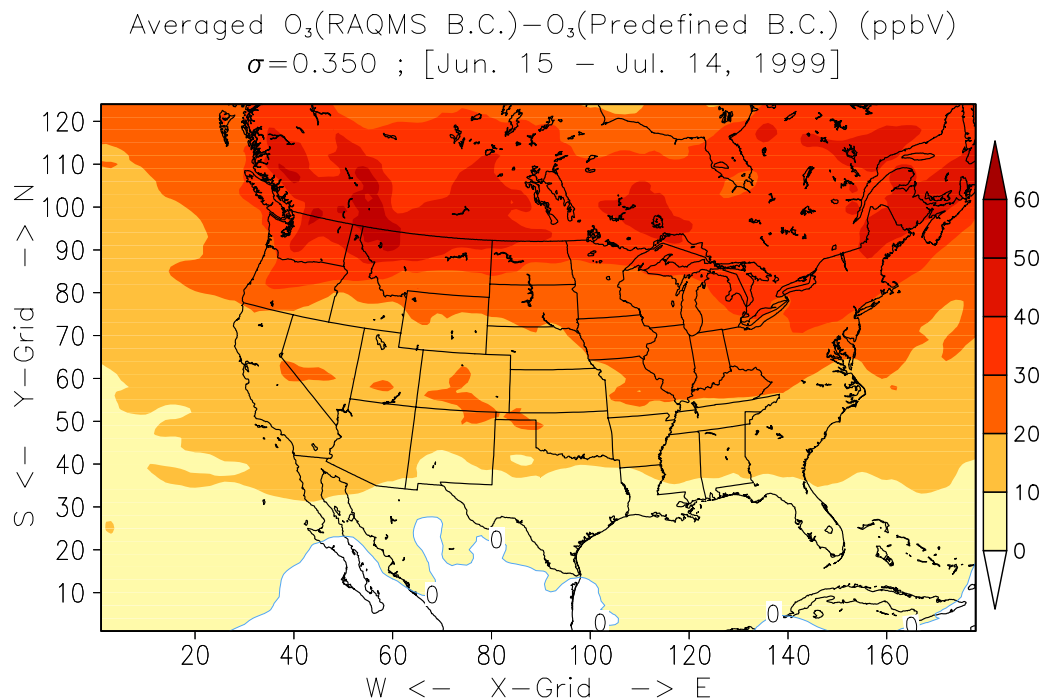


Figure 2b. Mean ozone differences (ppbv) between CMAQ/baseline and CMAQ/RAQMS observed in the upper troposphere ($\sigma = 0.350$). Average upper tropospheric differences of over 60 ppbv occur in the northern part of the domain, due to including the physically realistic cross-tropopause gradient in ozone from the RAQMS assimilated boundary conditions.



Comparisons of CMAQ with fixed boundary conditions, assimilated boundary conditions, AIRNow surface observations, and World Meteorological Organization ozonesonde data

In the following discussion, we compare CMAQ with fixed boundary conditions (baseline) with CMAQ using RAQMS assimilated boundary conditions (this study), and with “truth” (EPA AIRNow surface observations and World Meteorological Organization ozonesondes).

We evaluated the surface ozone concentrations (> 20 ppb) from CMAQ with two different boundary conditions: with default profile boundary conditions (CMAQ/baseline), and with the boundary conditions from RAQMS (CMAQ/RAQMS) by using a set of statistical analyses recommended by Willmott (1981). Table 1 shows that both of the CMAQ runs overestimated average surface ozone concentrations by 3 – 7 ppbv. The slope of regression line (b) is slightly less than 1, suggesting that the model underestimates peak ozone concentration during daytime, and overestimates lower ozone concentrations at nighttime.

Table 1. Averaged statistics for AIRNow surface ozone concentrations at 09 UTC (daytime) and 21 UTC (nighttime).

| | B.C. file | OBS. | | MODEL | | Regression | | | Bias | IOA | RMSE | Sys. RMSE | Unsys. RMSE | Skill_e | Skill_v | Skill_r |
|-----------|--------------|-------|-------|-------|-------|------------|-------|----------------|------|------|-------|--------------|----------------|---------|---------|---------|
| | | AVG | SD | AVG | SD | b | a | r ² | | | | | | | | |
| 09 UTC | Baseline | 34.66 | 12.59 | 39.24 | 10.64 | 0.85 | 9.93 | 0.13 | 4.58 | 0.60 | 14.00 | 12.03 | 4.97 | 0.96 | 0.85 | 1.11 |
| | RAQMS | 34.75 | 12.58 | 41.57 | 11.84 | 0.94 | 8.98 | 0.12 | 6.82 | 0.59 | 15.51 | 13.47 | 6.87 | 1.07 | 0.94 | 1.23 |
| 21 UTC | Baseline | 52.74 | 18.99 | 55.73 | 15.43 | 0.81 | 12.87 | 0.41 | 3.00 | 0.78 | 15.21 | 13.06 | 4.65 | 0.69 | 0.81 | 0.80 |
| | RAQMS | 52.80 | 18.97 | 58.11 | 16.69 | 0.88 | 11.73 | 0.42 | 5.31 | 0.78 | 16.04 | 14.02 | 5.79 | 0.74 | 0.88 | 0.85 |

Note: AVG=arithmetic average; SD=standard deviation; b=slope; a=intercept; IOA=index of agreement (close to 1 shows skill); Sys. RMSEs=systematic root mean square error; Unsys. RMSEu = unsystematic root mean square error; Skill_e = Unsys.RMSEu /observed SD (<1 shows skill); Skill_v = model SD/observed SD (close to 1 shows skill); Skill_r = RMSE/ observed SD (<1 shows skill).

Comparing surface ozone results from CMAQ/baseline, and CMAQ/RAQMS, the mean bias relative to AIRNow increased by about 2 ppbv in the CMAQ/RAQMS runs. The slopes of the regression lines improved by about 10 percent in the CMAQ/RAQMS runs. From these results, we estimate that the use of assimilated boundary conditions generated by RAQMS increased surface ozone concentrations about 2 ppbv over the baseline case, and increased (improved) the magnitude of the diurnal variation of surface ozone up to 10 % for study period. Similar evaluation statistics were generated for the several sub-regions (not presented here).

Next we compared ozone profiles from CMAQ/baseline and CMAQ/RAQMS, with World Meteorological Organization ozonesondes (“truth”) launched within the model domain during the study period. Table 2 lists the sampling sites available during the study.

Table 2. List of ozonesonde sites used for the comparison of CMAQ/ baseline and CMAQ/RAQMS boundary condition results.

| SITE # | Location | Nation | LAT. | LON. | ALT. |
|--------|----------------------|--------|-------|---------|---------|
| STN021 | EDMONTON/STONY PLAIN | CAN | 53.55 | -114.10 | 766.00 |
| STN076 | GOOSE BAY | CAN | 53.30 | -60.36 | 40.00 |
| STN077 | CHURCHILL | CAN | 58.75 | -94.07 | 35.00 |
| STN107 | WALLOPS ISLAND | USA | 37.90 | -75.48 | 13.00 |
| OH044 | OLD HICKORY | USA | 36.25 | -86.57 | 181.00 |
| ST67 | BOULDER | USA | 40.03 | -105.25 | 1634.00 |
| ST445 | TRINIDADHEAD | USA | 40.80 | -124.16 | 20.00 |

Figure 3 below compares CMAQ/baseline, CMAQ/RAQMS, and RAQMS analyses (no CMAQ) with observed ozone statistics for Canadian stations. This comparison with the Canadian ozonesondes indicates that using RAQMS assimilated boundary conditions from the global assimilation of satellite data significantly improves the performance of CMAQ in the upper troposphere in the northern part of the domain.

Figure 3. Comparison of CMAQ/baseline, CMAQ/RAQMS, and Canadian Ozonesonde Data (14 ozonesondes). Canadian ozonesonde data from Edmonton, Goose Bay, and Churchill stations. CMAQ/RAQMS performance matches ozonesondes better than CMAQ baseline. However, CMAQ/RAQMS performs less well than RAQMS_G, indicating that CMAQ introduces additional errors.

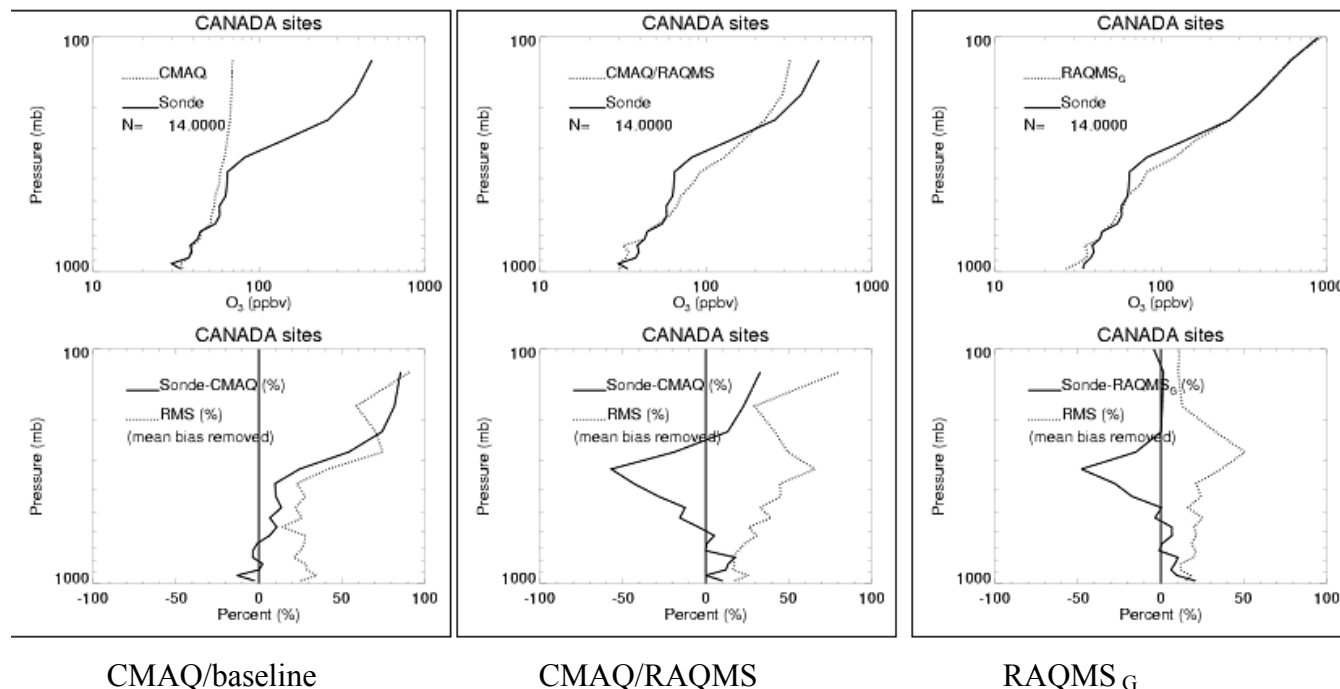
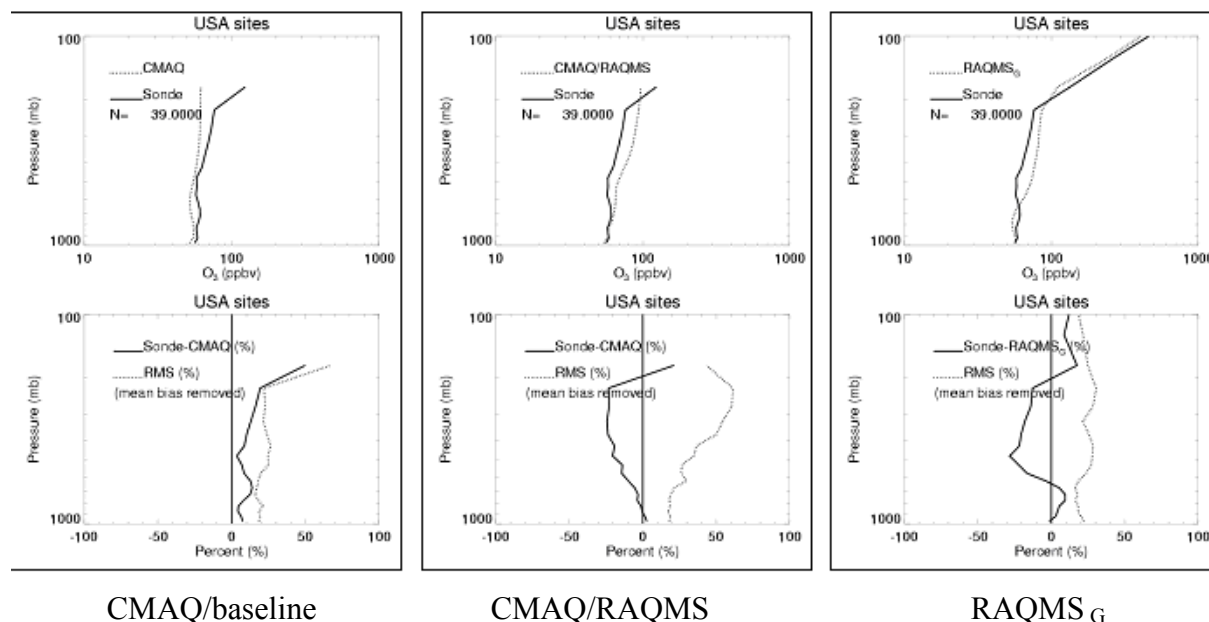


Figure 4 below compares CMAQ/baseline, CMAQ/RAQMS, and RAQMS analyses (no CMAQ) with observed ozone statistics for the USA stations. This comparison with the USA ozonesondes indicates that using RAQMS assimilated boundary conditions from the global assimilation of satellite data reduces (improves) the mean low biases above 600mb, but leads to increased RMS ozone errors above 600mb, relative to the CMAQ/baseline runs. For both Canadian and USA stations, the CMAQ/RAQMS mean ozone biases and RMS errors are larger than found in the RAQMS analyses without CMAQ above 600mb.

Figure 4. Comparison of CMAQ/baseline, CMAQ/RAQMS, and USA Ozonesonde Data (39 ozonesondes). USA ozonesonde data from Wallops Island, Boulder, and Old Hickory stations. CMAQ/RAQMS performance matches ozonesondes better than CMAQ baseline. However, CMAQ/RAQMS performs less well than RAQMS_G, indicating that CMAQ introduces additional errors.



The additional errors observed in the CMAQ/RAQMS runs (compared to the errors between RAQMS_G and ozonesondes, right panel) point to a degradation of the lateral boundary information constraints within the CMAQ interior domain in the mid to upper troposphere. The CMAQ model includes 5 layers between 500mb and the model top (100mb) with only one layer above 200mb. The RAQMS model uses 13 layers spanning this same region, with 7 of those layers lying above 200mb. These results indicate that improvements to the vertical resolution of CMAQ, and improvements in the convective exchange processes in the middle to upper troposphere may optimize benefits to CMAQ performance from using assimilated lateral boundary conditions.

Value of assimilated boundary conditions in CMAQ for large-scale ozone transport and surface ozone distributions

In the upper troposphere and lower stratosphere, the CMAQ (baseline) model failed to simulate the "chemical tropopause" above which ozone concentrations rapidly increase with height. On the other hand, the CMAQ/RAQMS results showed improved agreement with the ozonesondes in this region.

Comparisons with AIRNow surface ozone did not show significant differences between CMAQ/baseline and CMAQ/RAQMS at the surface.

These results indicate that using boundary conditions generated from global satellite data assimilation procedures improves the performance of CMAQ in the middle troposphere in the northern part of the U.S. continent and Canada.

Summary

- 1) The regional scale air quality model CMAQ was modified to accept assimilated lateral boundary conditions from the output of a global chemical model which assimilated global satellite-based ozone observations.
- 2) The fifty-five explicitly transported chemical species in RAQMS were mapped into those of the CMAQ CB4 mechanism, and interpolated onto the vertical levels of CMAQ.
- 3) Compared with the CMAQ baseline boundary conditions, CMAQ runs with the assimilated lateral boundary conditions from RAQMS showed a large difference in ozone concentration at the tropopause level in northern latitude regions, where the real-world (ozonesonde) concentration showed strong latitudinal gradients. The upper tropospheric ozone concentrations from CMAQ with the RAQMS boundary conditions showed increases of up to 200 ppbv compared to those with the CMAQ/baseline boundary conditions. CMAQ with the RAQMS boundary conditions is in better agreement with ozonesonde observations (100 – 400 ppbv).

Conclusion

This benchmark evaluated whether a multi-scale modeling and data assimilation framework for constraining global model predicts improved the prediction of large-scale transport and local productions of surface ozone and overall CMAQ performance. In the upper troposphere and lower stratosphere, the CMAQ/RAQMS results showed improved agreement with ozonesondes. CMAQ (baseline) model failed to simulate the "chemical tropopause" above which ozone concentrations rapidly increase with height. There were no significant differences in the surface distributions of ozone during the benchmark period between CMAQ/baseline and CMAQ/RAQMS.

The result of this benchmark was to identify that improvements to the vertical resolution of CMAQ, and improvements in the convective exchange processes in the middle to upper troposphere may optimize benefits to CMAQ performance from using assimilated lateral boundary conditions.

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Authorship

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Appendix A. Summary of mapping species between RAQMS and CMAQ CB4

CMAQ CB4

RAQMS

Nitrogen Species

| | | |
|-------------------------------|--|---|
| NO | Nitric oxide | NO_y-NO₂- NO_z* |
| | *) $\text{NO}_y = \text{N} + \text{NO} + \text{NO}_2 + \text{NO}_3 + 2(\text{N}_2\text{O}_5) + \text{HNO}_3 + \text{HNO}_4 + \text{BrNO}_3 + \text{ClNO}_3 + \text{PAN} + \text{ONIT} + \text{MPAN}$ | |
| | $\text{NO}_z^* = \text{NO}_3 + 2(\text{N}_2\text{O}_5) + \text{HNO}_3 + \text{HNO}_4 + \text{BrNO}_3 + \text{ClNO}_3 + \text{PAN} + \text{ONIT} + \text{MPAN}$ | |
| NO ₂ | Nitrogen dioxide | NO₂ |
| HONO | Nitrous acid | --- |
| | | (---: use the predefined profiles for B.C.) |
| NO ₃ | Nitrogen trioxide | NO₃ |
| N ₂ O ₅ | Nitrogen pentoxide | N₂O₅ |
| HNO ₃ | Nitric acid | HNO₃ |
| PNA | Peroxyntiric acid | HNO₄ |

Oxidants

| | | |
|-------------------------------|---|---|
| O ₃ | Ozone | O_x-NO₂- NO_z** |
| | **) $\text{O}_x = \text{O}(1\text{D}) + \text{O}(3\text{P}) + \text{O}_3 + \text{NO}_2 + \text{HNO}_3 + 2(\text{NO}_3) + 3(\text{N}_2\text{O}_5) + \text{HNO}_4 + \text{PAN} + \text{MPAN}$ | |
| | $\text{NO}_z^{**} = \text{HNO}_3 + 2(\text{NO}_3) + 3(\text{N}_2\text{O}_5) + \text{HNO}_4 + \text{PAN} + \text{MPAN}$ | |
| H ₂ O ₂ | Hydrogen peroxide | H₂O₂ |

Sulfur Species

| | | |
|-----------------|----------------|-----|
| SO ₂ | Sulfur dioxide | --- |
| SULF | Sulfuric acid | --- |

Atomic Species

| | | |
|-----|-----------------------|-----|
| O | Oxygen atom (triplet) | --- |
| O1D | Oxygen atom (singlet) | --- |

Odd Hydrogen Species

| | | |
|-----------------|---------------------|-----|
| OH | Hydroxyl radical | --- |
| HO ₂ | Hydroperoxy radical | --- |

Carbon oxides

| | | |
|----|-----------------|-----------|
| CO | Carbon monoxide | CO |
|----|-----------------|-----------|

Hydrocarbons

| | | |
|------|--|--|
| PAR | Paraffin carbon bond (C-C) | PAR+(10/4)C2H6+(1/3)PROP_PAR (PROP_PAR = propane paraffin, 1C) |
| ETH | Ethene (CH ₂ =CH ₂) | ETH |
| OLE | Olefinic carbon bond (C=C) | OLET (terminal olefin carbon group, 2C) |
| TOL | Toluene (C ₆ H ₄ -CH ₃) | --- |
| XYL | Xylene (C ₆ H ₅ -(CH ₃) ₂) | --- |
| ISOP | Isoprene | XISOP (Isoprene) |

Carbonyls and phenols

| | | |
|------|--|-------------|
| FORM | Formaldehyde | CH2O |
| ALD2 | Acetaldehyde and higher aldehydes | ALD2 |
| MGLY | Methyl glyoxal (CH ₃ C(O)C(O)H) | MGLY |
| CRES | Cresol and higher MW phenols | --- |

Organic nitrogen

| | | |
|-----|---|---|
| PAN | Peroxyacyl nitrate (CH ₃ C(O)OONO ₂) | PAN |
| NTR | Organic nitrate | ONIT (organic nitrate group, 2C) |

Organic Radicals

| | | |
|------|--|-----|
| C2O3 | Peroxyacyl radical (CH ₃ C(O)OO·) | --- |
| ROR | Secondary organic oxy radical | --- |
| CRO | Methylphenoxy radical | --- |

Operators

| | | |
|------|---------------------------------|-----|
| XO2 | NO-to-NO ₂ Operation | --- |
| XO2N | NO-to-nitrate operation | --- |

Products of organics

| | | |
|------|---------------------------------|--|
| TO2 | Toluene-hydroxyl radical adduct | --- |
| OPEN | High MW aromatic oxidation ring | --- |
| ISPD | Products of isoprene reactions | XMVK+XMACR+XISOPRD (XMVK = methyl vinyl ketone, 4C; XMACR = methacrolein; XISOPRD = isoprene oxidation product-long lived, 5C) |

Species added for aerosols

| | | |
|---------|---|-----|
| SULAER | Counter species for H ₂ SO ₄ production | --- |
| TOLAER | Counter species for toluene reaction | --- |
| XYLAER | Counter species for xylene reaction | --- |
| CSLAER | Counter species for cresol reaction | --- |
| TERPAER | Counter species for terpene reaction | --- |
| TERP | Monoterpenes | --- |

Species added for aqueous chemistry

| | | |
|------|------------------------------------|-----|
| FACD | Formic acid | --- |
| AACD | Acetic and higher acids | --- |
| PACD | Peroxy acetic acid | --- |
| UMHP | Upper limit of methylhydroperoxide | --- |

Unused species (RAQMS)**Cl**

Cl_y; HCl; ClONO₂; OCIO; CCl₄; CH₃Cl; CH₃CCl₃; HOCl; Cl₂

Br

Br_y; CH₃Br; HBr; BrONO₂; HOBr;

F

HF; CF₂O;

Cl+Br+F

CFCI₃; CF₂Cl₂; CF₃Br; CF₂ClBr; CFCIO; BrCl

etc

CH₄; H₂O; N₂O; ETHOOH (ethyl hydrogen peroxide, 2C); ROOH (C₃+hydrogen peroxide group, 1C), CH₃OH (methanol)